

Effect of the Tottori familial disease mutation (D7N) on the monomers and dimers of A β 40 and A β 42

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Table S1: Relative rate of fibril formation (RRFF) upon D7N mutation using the $\text{A}\beta_{40}$ and $\text{A}\beta_{42}$ monomers and dimers.

	$\text{A}\beta_{40}$		$\text{A}\beta_{42}$		2 $\text{A}\beta_{40}$		2 $\text{A}\beta_{42}$	
	22-28	23-28	22-28	23-28	22-28	23-28	22-28	23-28
RFFF	0.03	12.5	3.4	2.2	1.6	1.0	9.3	11.3

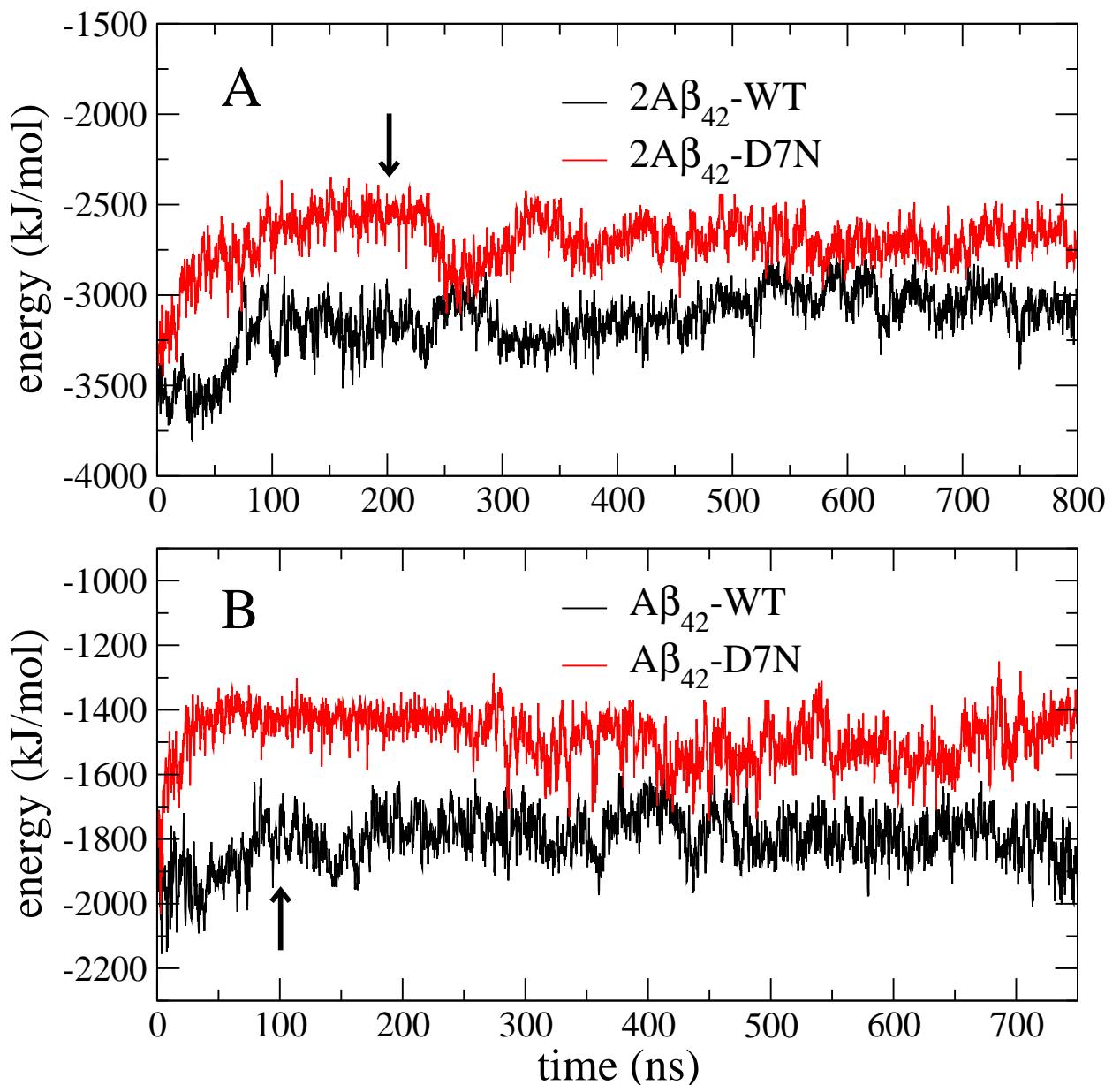


Fig. S1: Potential energies of the dimeric (A) and monomeric (B) $\text{A}\beta_{42}$ systems. The energies include the protein-protein and protein-solvent contributions. The arrows indicate the time where the energy has equilibrated. The same equilibration time of 100 ns is observed for the $\text{A}\beta_{40}$ monomers, while it is 250 ns for the $\text{A}\beta_{40}$ dimers

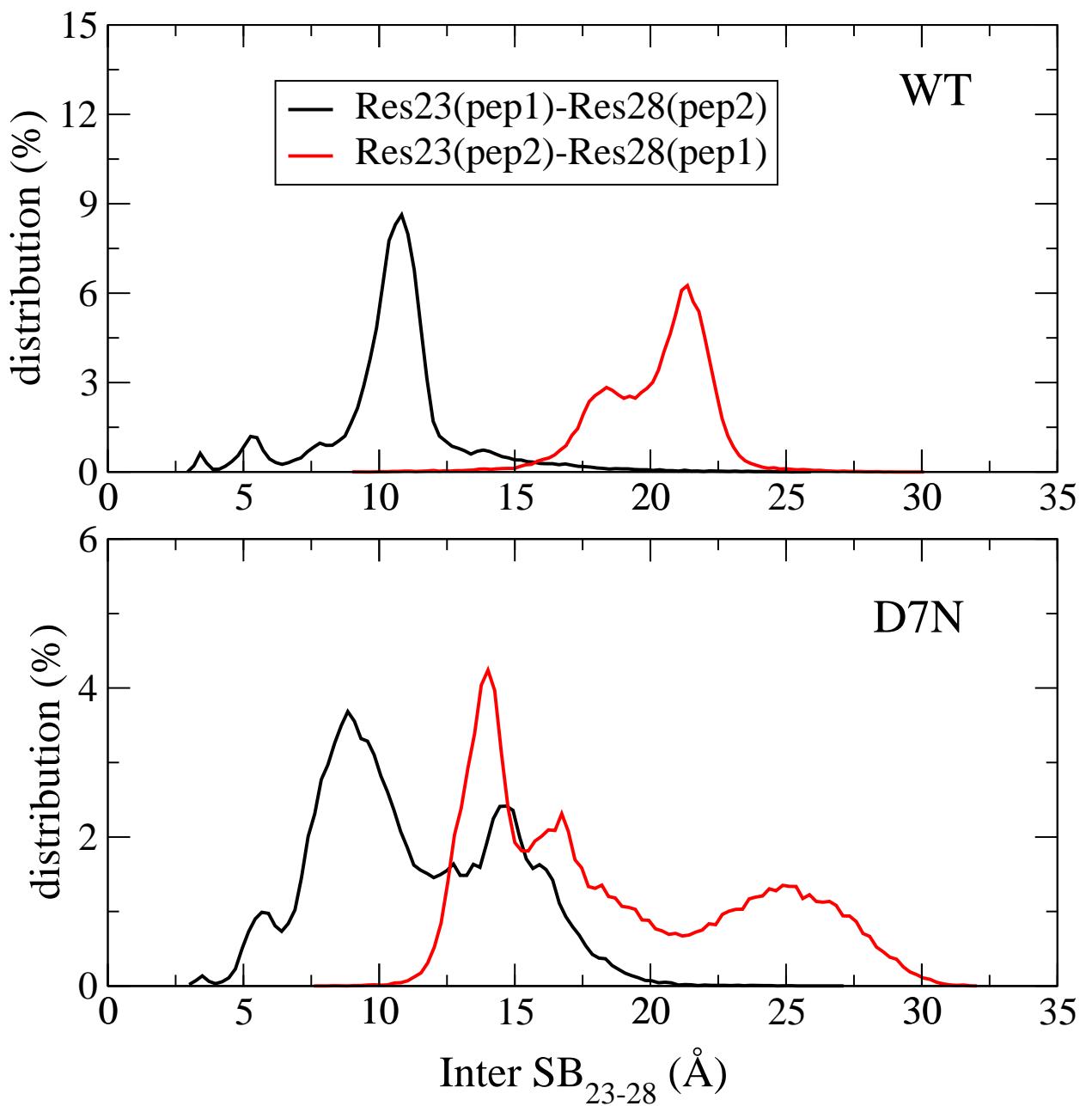


Fig. S2: The population of the intermolecular 28-23 salt bridge distances in the $\text{A}\beta_{42}$ dimers. Pepi refers to the chain number. The data are obtained using 900 ns.

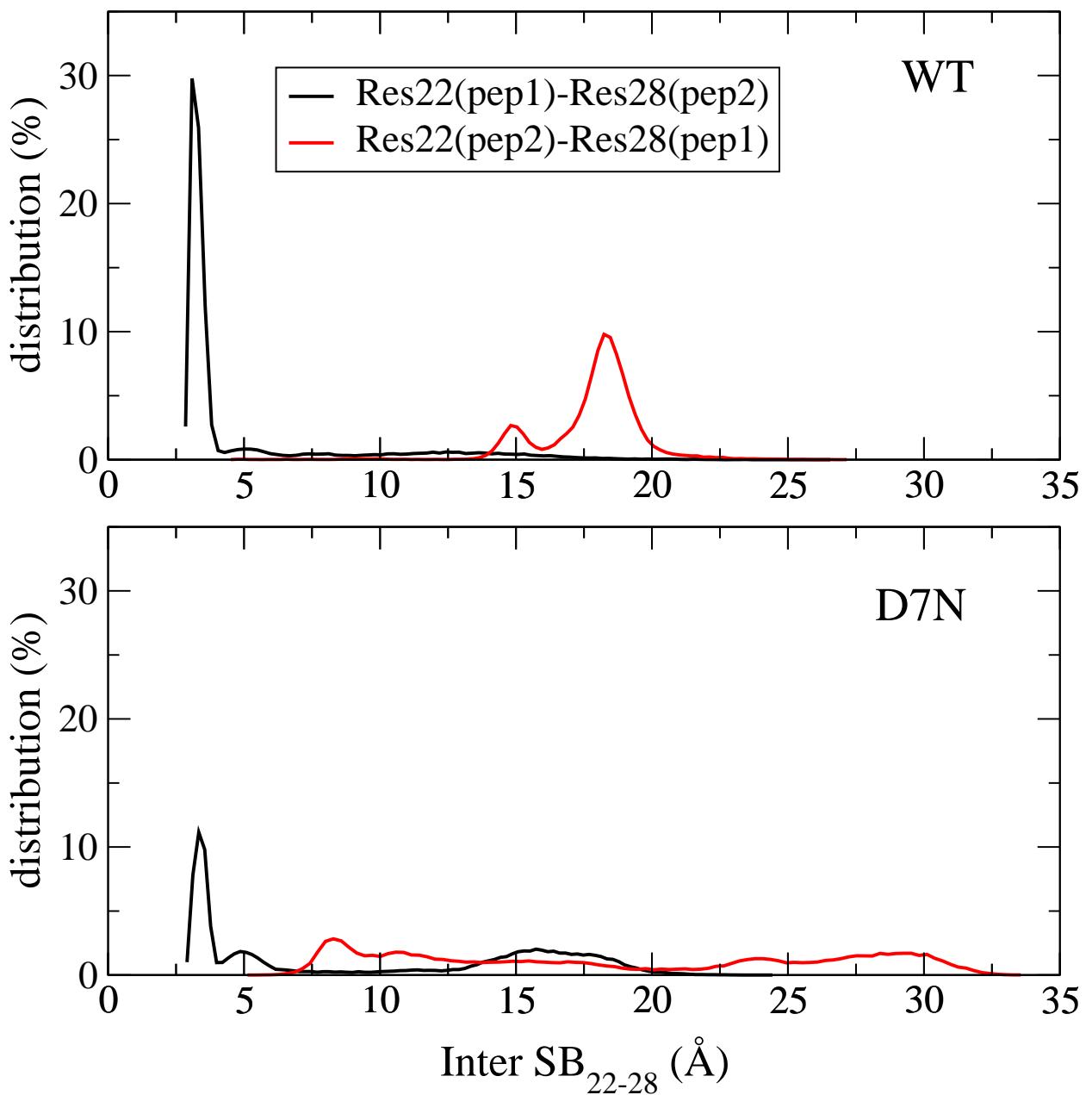


Fig. S3: The population of the intermolecular 28-22 salt bridge distances in the A β ₄₂ dimers. Pepi refers to the chain number. The data are obtained using 900 ns.

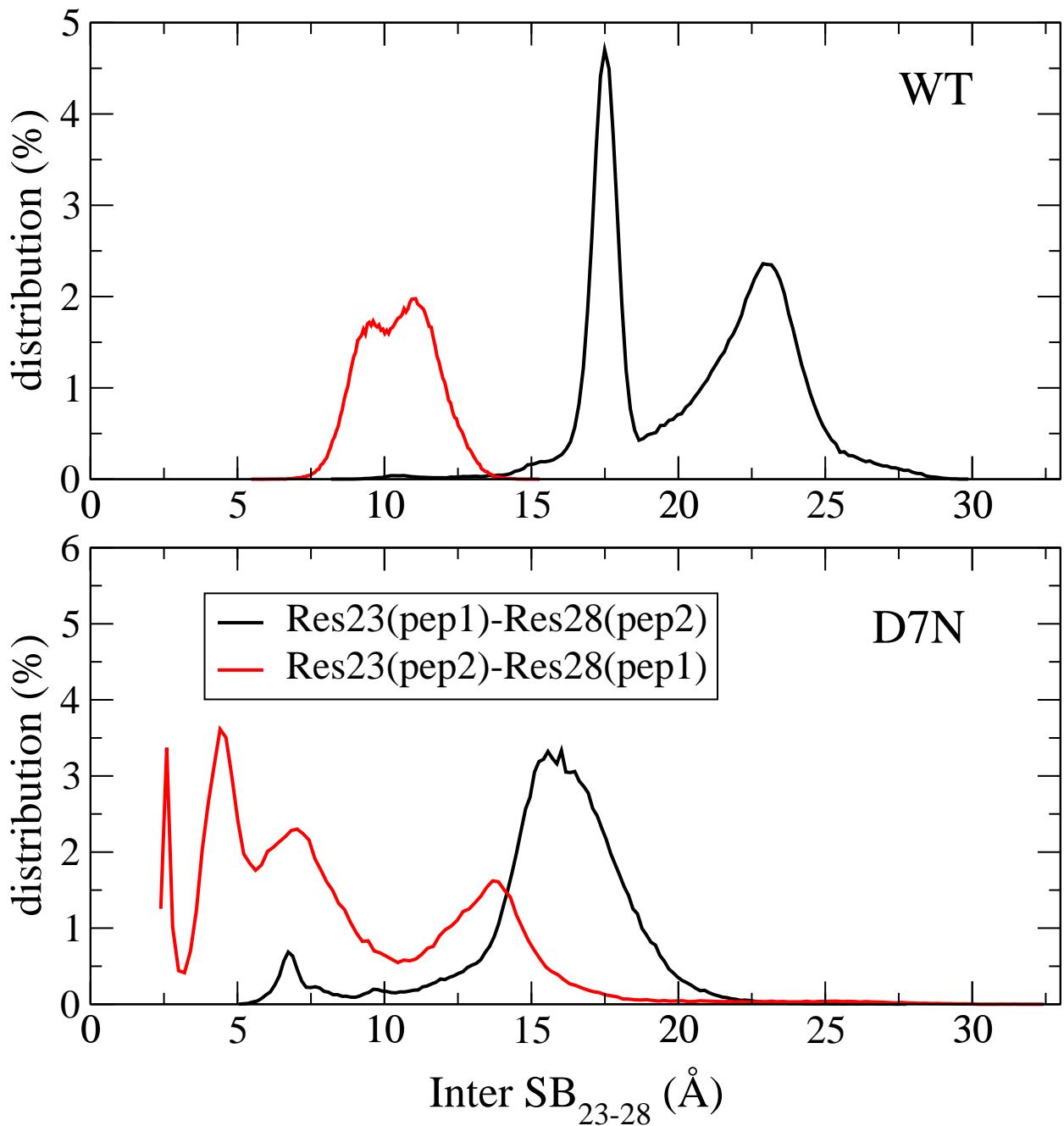


Fig. S4: The population of the intermolecular 28-23 salt bridge distances in the A β ₄₀ dimers. The data are obtained using 950 ns.

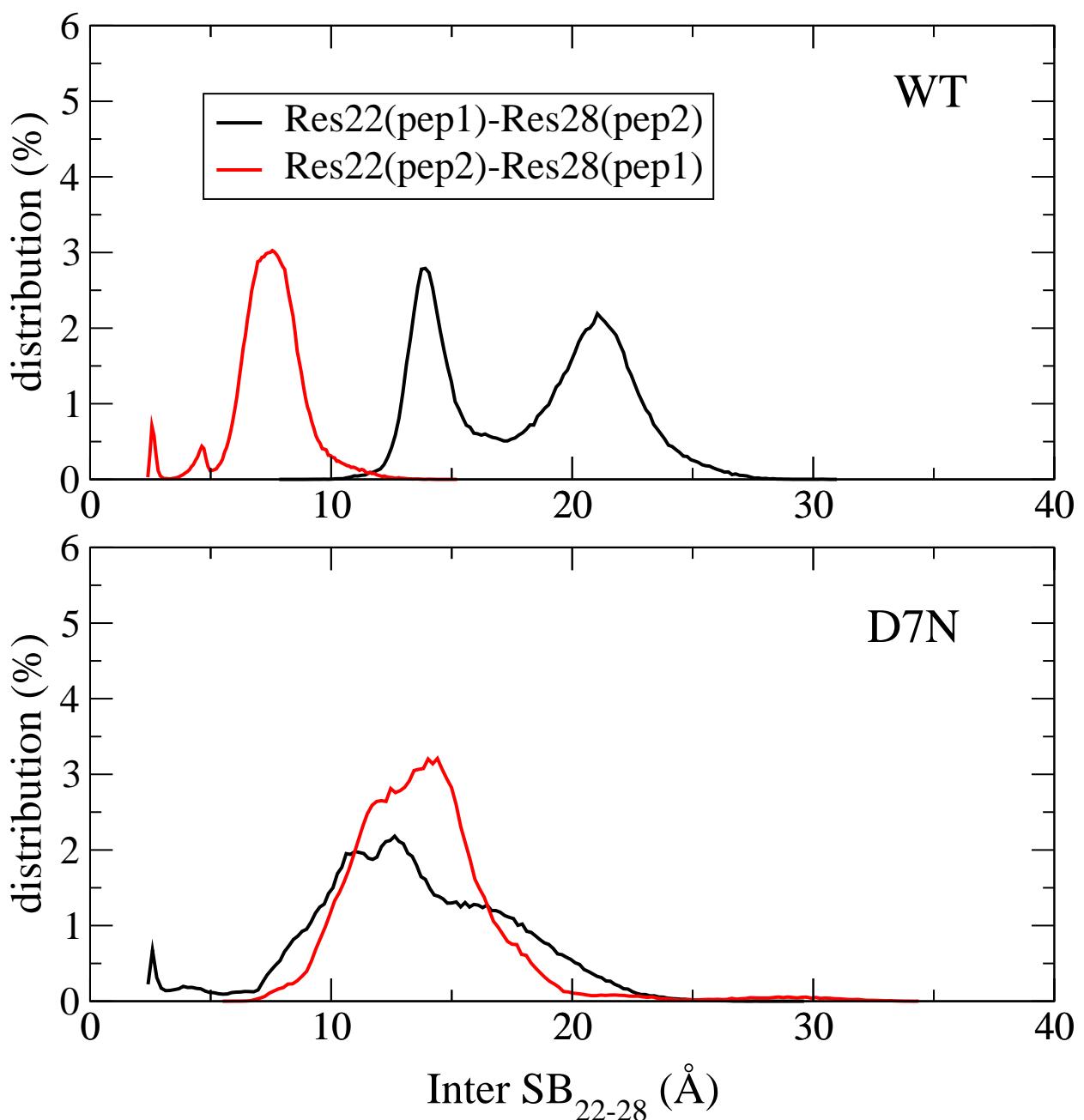


Fig. S5: The population of intermolecular 28-22 salt bridge distances in the $\text{A}\beta_{40}$ dimers. The data are obtained using 950 ns.

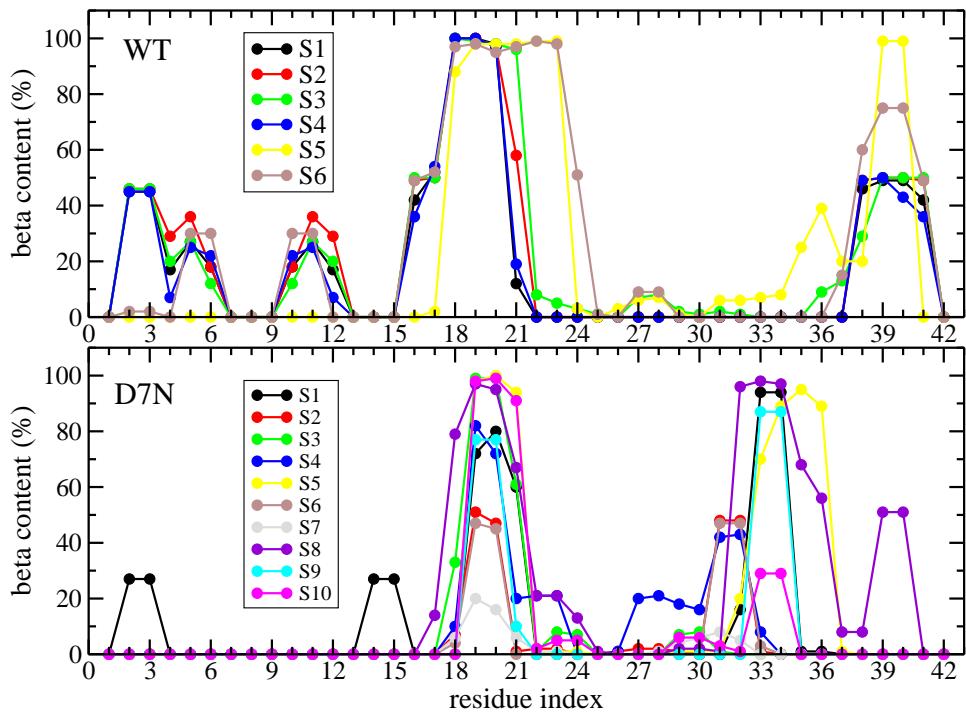


Fig. S6: Averaged β content (%) along the amino acid sequence for the conformations belonging to the states S_i shown on the free energy landscapes of the $A\beta_{42}$ dimers. The data are obtained using using the full 800 ns simulation and 300 ns from 6 MD simulations.

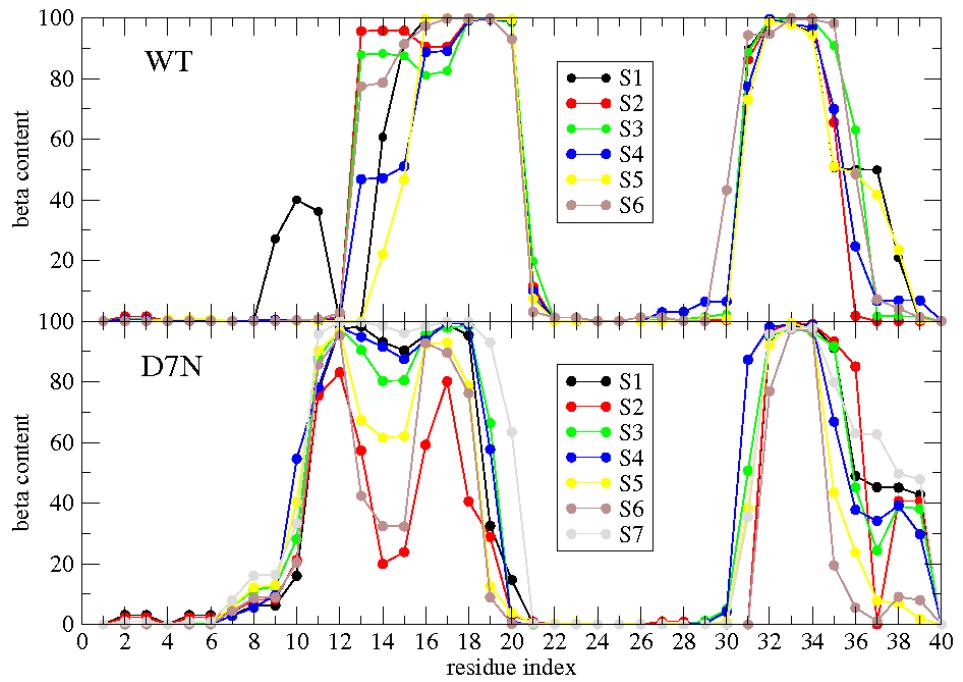


Fig. S7: Averaged β content (%) along the amino acid sequence for the conformations belonging to the states S_i shown on the free energy landscapes of the $A\beta_{40}$ dimers. The data are obtained using the full 850 ns simulation and 300 ns from 6 MD simulations.